

CONTENTS

Preface	V
Contributors to this volume	IX
Part I. Computational models	
A.J. SADLEJ - Computational quantum chemistry: advances, perspectives and limitations	3
L.A. GRIBOV - Basic problems of computation of molecular optical spectra	32
M. MARSILI and J. GASTEIGER - Fast calculation of atomic charges from molecular topology and orbital electronegativities	56
P.A.D. deMAINE - Automatic methods for designing experiments and processing data	68
L. EDSBERG - Implementation of programs for interactive simulation of chemical kinetics	79
L. EDSBERG - Some numerical problems in mathematical models for chemical kinetics	88
J.W. KENNEDY - Small graphs, graph theory and chemistry	96
J.W. KENNEDY - Statistical mechanics and large random graphs	115
H.J. HARWOOD - Use of computers for calculating structural features of polymers	133

Part II. Morphological models

J.T. CLERC and H. KOENITZER - Storage and retrieval of spectroscopic data	151
S.R. HELLER - The development and evolution of a chemical information system	164
S. SASAKI, H. ABE, I. FUJIWARA and T. YAMASAKI - The application of ¹³ CNMR in CHEMICS, the computer program system for structure elucidation	186

Part III. Semantic models

Z. HIPPE, O. ACHMATOWICZ Jr. and R. HIPPE - Some problems of computer-aided discovery of organic syntheses ..	207
I. UGI, J. BAUER, J. BRANDT, J. DUGUNDJI, R. FRANK, J. FRIEDRICH, A. von SCHOLLEY and W. SCHUBERT - Mathematical model of constitutional chemistry and system of computer programs for deductive solution of chemical problems	219
J. GASTEIGER, M. MARSILI and B. PAULUS - Investigations into chemical reactivity and planning of chemical syntheses	229

Part IV. Various topics

Z. HIPPE - Manipulation of chemical structures within a computer	249
E. STEGER and K. HERZOG - Performance of infra-red spectrometers directly coupled to computers	259
A.M. JANICKI - Recent trends in development of computer system architecture required by characteristic features of chemical researches	276